

Exactly solvable spin chain models corresponding to BDI class of topological superconductors

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We present an exactly solvable extension of the quantum XY chain with longer range multi-spin interactions. Topological phase transitions of the model are classified in terms of the number of Majorana zero modes, n_M which are in turn related to an integer winding number, n_W . The present class of exactly solvable models belong to the BDI class in the Altland-Zirnbauer classification of topological superconductors. We show that time reversal (TR) symmetry of the spin variables translates into a *sliding* particle-hole (PH) transformation in the language of Jordan-Wigner (JW) fermions – a PH transformation followed by a π shift in the wave vector (π PH). Presence of π PH symmetry restricts the n_W (n_M) of TR symmetric extensions of XY to odd (even) integers. The π PH operator may serve in further detailed classification of topological superconductors in higher dimensions as well.

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The spectrum of Quantum XY model is exhausted by the emergent JW fermions^{1,2}. The anisotropy of the exchange coupling generates p-wave superconducting pairing between spinless JW fermions leading to unpaired Majorana fermion (MF) at ends of an open chain³. Adding further neighbor XY couplings in general spoils the exact solvability because the JW transformation incorporates appropriate (non-local) phase strings in order to fulfill anti-commutation algebra². In the context of the Ising in a transverse field (ITF) model it was recently shown that adding appropriately engineered three-spin interactions can still leave it exactly solvable⁴. Given that ITF and XY model are related by a duality transformation^{5,6} we expect similar extensions to work for the XY model. In this letter we classify generalizations of the XY model with arbitrary n -spin interactions in terms of a π PH symmetry that is a PH transformation followed by a sign alternation in one sublattice. We show that in presence of π PH corresponding to every MF there will be a partner MF which will correspondingly restrict the possible winding numbers. Let us start with the XY Hamiltonian,

$$H_{XY} = \sum_j (J_1 + \lambda_1) \sigma_j^x \sigma_{j+1}^x + \sum_j (J_1 - \lambda_1) \sigma_j^y \sigma_{j+1}^y, \quad (1)$$

to which we add a n -spin interaction,

$$H_{nXY} = H_{XY} + \sum_{j,a} (J_r + \eta_a \lambda_r) \sigma_j^a \left(\prod_{k=1}^{r-1} \sigma_{j+k}^z \right) \sigma_{j+r}^a, \quad (2)$$

where $a = x, y$ and $\eta_x = -\eta_y = 1$. Here $r = n - 1$ denotes the range of n -spin interaction. J_r is the longer range exchange and λ_r denotes the longer range XY anisotropy. For this Hamiltonian (nXY model) the quantity $q = \prod_{\ell=1}^N \sigma_{\ell}^z$ is a constant of motion. Two possible $q = \pm 1$ values correspond to number parity of JW fermions and hence the above generalization is expected to give a superconducting system. Indeed the JW transformation²,

$$\sigma_j^z = 1 - 2c_j^\dagger c_j, \quad \sigma_j^x = e^{i\phi_j} (c_j + c_j^\dagger), \quad \sigma_j^y = -ie^{i\phi_j} (c_j - c_j^\dagger), \quad (3)$$

where ϕ_j is the phase string defined as $\phi_j = \pi \sum_{\ell < j} c_\ell^\dagger c_\ell$ converts the above Hamiltonian to,

$$H = 2 \sum_{s=1,r} \sum_j (J_s c_j^\dagger c_{j+s} + \lambda_s c_j c_{j+s} + \text{h.c.}), \quad (4)$$

where longer range exchange and anisotropy parameter J_s, λ_s give rise to hopping and pairing between s 'th neighbors, respectively. Note the important role played by σ^z phases is to cancel the unwanted JW phases which renders the nXY Hamiltonian to the quadratic form (4).

For even (odd) r the generalized term involves $n = r + 1$ spins which will be odd (even) under the TR. Let us now figure out how does the JW dictionary translate the TR operation of spin variables. The TR changes the sign of spin operators $\vec{\sigma}_j$. Sign reversal of σ_ℓ^z with $\ell < j$ implies that under TR the non-local phase string is transformed as $e^{i\phi_j} \rightarrow (-1)^{j-1} e^{i\phi_j}$. Therefore the TR of spins for JW fermions translates to,

$$c_j \rightarrow (-1)^{j-1} c_j^\dagger \Leftrightarrow c_k \rightarrow -c_{\pi-k}^\dagger \quad (5)$$

which is nothing but the PH transformation followed a π shift in the k -space – or *sliding* PH – that will be denoted by π PH in this paper. The π PH can further resolve the topological classification of the Altland-Zirnbauer (AZ) classification of topological superconductors⁷ that are based on PH, TR, and sublattice symmetries⁸⁻¹¹. In the following we discuss in detail two prototypical cases corresponding to longer range interaction with range $r = 2, 3$ involving $n = 3, 4$ spins, respectively. Then we present general arguments for arbitrary r and discuss an even-odd dichotomy related to the π PH transformation.

3XY Model. In this case the k -space representation of the JW Hamiltonian is,

$$H = \sum_k \mathbf{c}_k^\dagger \vec{h}_k \cdot \vec{\tau} \mathbf{c}_k, \quad \mathbf{c}_k^\dagger = (c_k^\dagger, c_{-k}) \quad (6)$$

where τ^a , $a = x, y, z$ stands for Pauli matrices in the Nambu space and $\vec{h}(k) = \varepsilon_k \hat{z} + \Delta_k \hat{y}$ with

$$\varepsilon_k = J_1 \cos k + J_2 \cos 2k, \quad \Delta_k = -\lambda_1 \sin k - \lambda_2 \sin 2k. \quad (7)$$

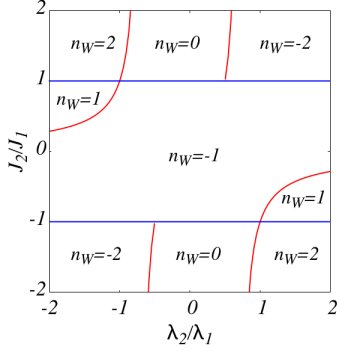


FIG. 1. (Color online) The phase diagram of 3XY model in parameter space. The phase boundary curves correspond to gap closing separating topologically distinct phases characterized by a winding number n_W as indicated in the figure.

Note that pairing with (hopping to) a neighbor at distance $r = 2$ has added a $\lambda_2 \sin 2k$ ($J_2 \cos 2k$) term to the Anderson pseudovector \tilde{h} representation of the Hamiltonian matrix. This general feature holds for any r . The eigenvalues and eigenvectors of $\tilde{h}(k)$ are given by,

$$E_k = \pm \sqrt{\varepsilon_k^2 + \Delta_k^2}, \quad |\psi_k^-\rangle = \begin{pmatrix} iu_k \\ v_k \end{pmatrix}, \quad |\psi_k^+\rangle = \begin{pmatrix} v_k \\ iu_k \end{pmatrix}, \quad (8)$$

where the coherence factors are parameterized in terms of a phase $\phi_k = \tan^{-1}(\Delta_k/(\varepsilon_k + E_k))$ as $u_k = \sin(\phi_k/2)$ and $v_k = \cos(\phi_k/2)$. The JW Hamiltonian (6) is diagonalized in terms of Bogolons $\gamma_k^\dagger = -iu_k c_k^\dagger + v_k c_{-k}$.

The boundaries of the phase diagram of the 3XY model can be analytically calculated by investigating the gap closing of the spectrum (8) that happens when both ε_k and Δ_k vanish which gives following equations for the phase boundaries,

$$\frac{J_2}{J_1} = \pm 1, \quad \text{or} \quad \frac{J_2}{J_1} = \frac{(\lambda_2/\lambda_1)}{1 - 2(\lambda_2/\lambda_1)^2} \quad \text{for} \quad \left| \frac{\lambda_2}{\lambda_1} \right| \geq 1/2, \quad (9)$$

which has been plotted in Fig. 1. It is remarkable that the phase boundary is given in terms of ratios J_2/J_1 and λ_2/λ_1 . This property is also general and the phase diagram is determined only in terms of the ratios J_r/J_1 and λ_r/λ_1 . In Fig. 1 each region is labeled by a winding number n_W . This topological invariant corresponds to the number of times the unit circle is covered by the vector $(\Delta_k, \varepsilon_k)$ as k varies across the first Brillouin zone (1BZ)¹². These vectors are represented by black arrows in Fig. 2 which correspond to green curve representing ϕ_k/π . The winding pattern of arrows and the global variation profile of ϕ_k does not change as long as the phase boundaries of Fig. 1 are not crossed. This means that n_W is a topological invariant¹³. For the 3XY model five possible values $n_W = 0, \pm 1, \pm 2$ can be extracted from analysis similar to Fig. 2. The resulting n_W values are used to label regions of Fig. 1. The phase with $n_W = 0$ is adiabatically connected to the trivially gapped phase that can be reached by an applied field $h \rightarrow \pm\infty$ that couples to σ^z without gap closing. This makes the $n_W = 0$ region topologically trivial. This is while

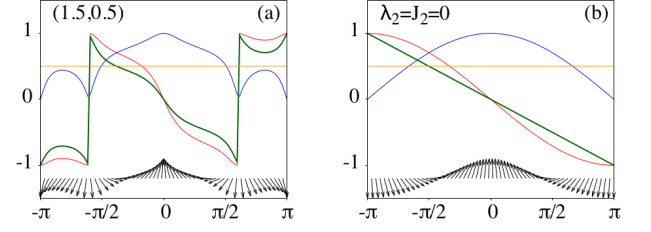


FIG. 2. (Color online) Wave function and winding pattern for representative points in regions various phases of Fig. 1. The red and blue curves represent the coherence factors u_k and v_k as a function of k and the green curve corresponds to the ϕ_k/π . Black arrows are unit vectors constructed from Anderson pseudovector $(\Delta_k, \varepsilon_k)$ at every k in the 1BZ. The coordinate $(\lambda_2/\lambda_1, J_2/J_1)$ is shown in the top left of each panel. The resulting n_W is used to label regions of Fig. 1.

the other phases with $n_W \neq 0$ are separated from the trivially gapped phase by a gap closing. The panel (b) of Fig. 2 corresponds to $\lambda_2 = J_2 = 0$ where $\lambda_1 \neq 0$ is adiabatically connected to the Ising limit $\lambda_1 = 1$. This is why the phase boundary (9) is determined by the ratio λ_2/λ_1 .

Let us show that for any r the nXY model falls into BDI class⁸ which in turn allows for winding number classification. First let us check the TR symmetry. For spinless fermions TR operator \mathcal{T} is simply a complex conjugation. Using the Nambu space representation, Eq. (6), we have $\mathcal{T}\tilde{h}(k)\mathcal{T} = \tilde{h}(-k)$ which represents the TR symmetry of the JW Hamiltonian. Now defining the operator $\mathcal{C} = \tau_x K$ as the PH transformation, one finds $\mathcal{C}\tilde{h}(k)\mathcal{C} = -\tilde{h}(k)$ that checks the PH symmetry. Finally for the chiral symmetry we have, $\tilde{h}(k)\mathcal{C}\mathcal{T} = -\mathcal{C}\mathcal{T}\tilde{h}(k)$. Let us emphasize that for every r , only $\sin(rk)$ functions appear in the pairing term and hence the above properties that rest on odd parity of Δ_k apply to nXY model. Since for the present spinless JW fermions one has $\mathcal{C}^2 = \mathcal{T}^2 = +1$, the nXY belongs to BDI class in the AZ classification of topological superconductors and hence allows for integer (winding number) classification of the topological phases. However both range of possible integers and whether they are even or odd is determined by r which in turn is connected to the presence or absence of the sliding PH symmetry, π PH. To set the stages for discussion of arbitrary r , let us consider the next prototypical case of 4-spin interactions.

4XY Model. The four-spin term preserves the TR symmetry of the spin model. The components of Anderson pseudovector are given by, $\varepsilon_k = J_1 \cos(k) + J_2 \cos(3k)$ and $\Delta_k = \lambda_1 \sin(k) + \lambda_2 \sin(3k)$. The phase boundaries will be given by setting $\varepsilon_k = \Delta_k = 0$. Therefore the gap closing curves of this model are the lines $\lambda_2/\lambda_1 = 1$ and $J_2/J_1 = -1$, and the curve

$$\frac{\lambda_2}{\lambda_1} = 1, \quad \text{or} \quad \frac{J_2}{J_1} = -1, \quad \text{or} \quad \frac{J_2}{J_1} = \frac{\lambda_2/\lambda_1}{1 + 2\lambda_2/\lambda_1}, \quad (10)$$

for $\lambda_2/\lambda_1 \geq 1$ and $\lambda_2/\lambda_1 \leq -1/3$. These curves partition the parameter space $(\lambda_2/\lambda_1, J_2/J_1)$ into seven regions represented in the right panel of Fig. 3 each characterized by $n_W = \pm 1, \pm 3$. The left panel of this figure represents same

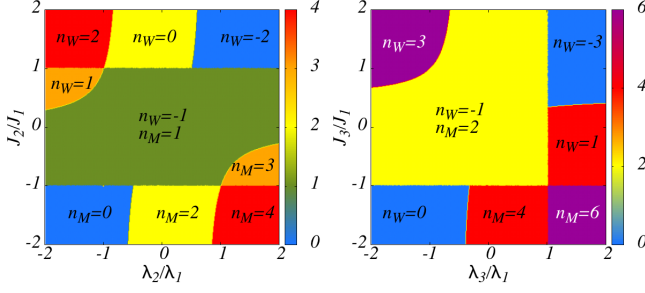


FIG. 3. (Color online) Color map of the number of MFs, n_M in the parameter space for two extensions 3XY (left) and 4XY (right) corresponding to spin clusters of range $r = 2, 3$, respectively. The 4XY model has π PH symmetry in JW representation which restricts n_M to even values and n_W to odd values only. Obviously the origin in both cases correspond to $r = 1$ which is not continuously connected to topologically distinct cases of $r = 2$ (left) nor $r = 3$ (right).

set of data for 3XY model. In both $r = 2, 3$ cases $|n_W| \leq r$ while for odd r only odd values of n_W are picked. To explain the meaning of the color code in this figure, let us discuss the number n_M of MFs for a general r .

Majorana end modes. To further understand the properties of nXY model, let us now consider an open nXY chain and discuss the Majorana zero modes of the chain. Presence of MFs requires equal spin (or spinless pairing)^{12,14} which engineered in one¹⁵ or two¹⁶ dimensions. In the case of XY models the spinless pairing emerges³. Let us now see how do MFs appear in nXY model. In terms of MFs $a_j = c_j + c_j^\dagger$, $b_j = i(c_j - c_j^\dagger)$ the nXY model becomes,

$$H = i \sum_{s=1, r} \sum_j (J_s + \lambda_s) a_j b_{j+s} + (\lambda_s - J_s) b_j a_{j+s}. \quad (11)$$

We search for MFs of type a localized near the origin for the nXY model, i.e. zero-energy states of the form $(A_1, 0, A_2, \dots, A_N, 0)$ with $A_j \sim x^j$ which gives,

$$(J_r + \lambda_r) + (J_1 + \lambda_1)x^{r-1} - (\lambda_1 - J_1)x^{r+1} - (\lambda_r - J_r)x^{2r} = 0. \quad (12)$$

If we search for solutions of type $(0, B_1, \dots, 0, B_N)$, we would obtain a similar equation but with $x \rightarrow x^{-1}$. To have a normalizable Majorana zero mode of type a we need solutions that satisfy $|x| < 1$. Fig. 3 represents a color map of the number n_M of MFs of type a localized in one end for $r = 2, 3$. The first thing to note is that the phase boundaries in the 3XY model obtained from the MF counting analysis precisely coincides with that in Fig. 1. This is also true for the 4XY model, and the boundaries given by Eq. (10) precisely coincide with that in the right panel of Fig. 3. The color code in each panel of this figure indicates the number of MFs of type a bound to left end. For each panel we have explicitly indicated n_W . It can be observed that in both cases,

$$n_W = n_M - r \quad (13)$$

where r is the range of interaction. Let us present a heuristic argument that the above formula holds for any r .

To proceed further let us first elucidate the meaning of π PH in the language of MFs: If we represent the JW "electron" and "hole" operators as $c_j^\dagger = a_j + ib_j$ and $h_j = a_j' - ib_j'$ and if we search for MFs with vanishing b, b' component, then every zero mode solution $(A_1, 0, A_2, 0, \dots)$ is mapped by π PH to a partner MF $(A_1', 0, A_2', 0, \dots)$ with $A_j' = -(-1)^j A_j$.

For even values of r where odd number of spin variables are added to the XY model, consider any point in the phase diagram (see left panel of Fig. 3) with given number n_M of MFs. Obviously the generalized $r + 1$ -spin interaction breaks TR symmetry. In this case the overall minus arising from TR transformation can be absorbed by the transformation $(\lambda_r, J_r) \rightarrow -(\lambda_r, J_r)$. This means that for every MF at point $(\lambda_1, J_1, \lambda_r, J_r)$ of the phase diagram, its partner MF corresponds to point $(\lambda_1, J_1, -\lambda_r, -J_r)$. This explains the inversion symmetry in the left panel of Fig. 3. This can also be seen from Eq. (12) that maps to itself under simultaneous change of $x \rightarrow -x$ and $(\lambda_r, J_r) \rightarrow -(\lambda_r, J_r)$. For odd values of r , there are even number of spins giving a TR symmetric term and hence the TR operation does not produce any minus sign in the n -spin term. Therefore corresponding to every MF at any point $(\lambda_1, J_1, \lambda_r, J_r)$, the partner MF also exists at the same point in the parameter space. This can also be seen directly from Eq. (12): Although in general Eq. (12) admits $2r$ solutions such that the number n_M of them satisfying $|x| < 1$ is $0 \leq n_M \leq 2r$. However, for odd r this equation becomes an equation of degree r in terms of $X = x^2$ which implies that the solutions always come in pairs $\pm x$ giving partner MFs as $A_j \sim (\pm x)^j$. This explains why in the right panel of Fig. 3 only colors corresponding to even n_M appear. The presence of π PH for odd r implies that corresponding to every MF at the chain end, its partner obtained by sign alternation in one-sublattice is also acceptable solution and hence n_M is always even. Now let us discuss how does π PH restrict n_W .

Consider an arbitrary point in the phase diagram corresponding to pairing amplitudes $\{\lambda_s\}$. Since the resulting JW Hamiltonian (4) is TR symmetric, the action of TR is simply $i \rightarrow -i$ which can be absorbed by $\{\lambda_s\} \rightarrow \{-\lambda_s\}$. The later on other hand amounts to changing the sign of the horizontal component Δ_k of the Anderson pseudovector. Therefore it is the implication of TR symmetry of JW Hamiltonian that corresponding to every winding number n_W , there is a winding number $-n_W$ irrespective of whether r is even or odd. Now let us argue that the possible values of n_W are bounded by the range r of interaction. Every time Δ_k vanishes, the pseudovector points vertically either to the south or north pole. For the nXY model the maximum number of the zeros of Δ_k in the 1BZ produced by combination first and r 'th harmonics of sin function is r which implies $|n_W| \leq r$.

To see when the maximum number of zeros in Δ_k are realized, it is enough to consider the limit $J_r \sim r\lambda_r \gg \lambda_1 \sim J_1$ where there are $2r + 1$ zeros for Δ_k in the 1BZ which give maximal winding $|n_W| = r$. In this limit the secular equation (12) reduces to $x^{-2r} = (r - 1)/(r + 1)$ the absolute value of which is always less than unity for every $r > 0$ which realizes maximum number of MFs equal to $2r$. This means that the maximum values of n_W and n_M happen in the same limit. Now the point with minimum n_W is the TR of

the maximal n_W . The TR for JW Hamiltonian is equivalent to $\{\lambda_s\} \rightarrow \{-\lambda_s\}$ which is a $\pi/2$ rotation around the z -axis for spin variables and the operation $a \leftrightarrow b$ for MFs which essentially exchanges $x \leftrightarrow x^{-1}$ and hence mapping every state with n_M MFs to a state with $2r - n_M$ MFs. Therefore both upper and lower bounds of $2r + 1$ possible integers $|n_W| \leq r$ and $0 \leq n_M \leq 2r$ describe the same physical state. Finally, since both n_M and n_W are unique topological labels of the same state, the mapping between the two sets must be one-to-one. Since the ends of two chains of integers map to each other, we heuristically expect Eq. (13) to hold for any r .

Now let us discuss why for odd values of $r = 2p + 1$ the n_W is always odd. The n_W changes by half between each two consecutive zeros of $\Delta_k = \lambda_1 \sin k + \lambda_r \sin((2p + 1)k)$. Suppose that this gap function vanishes at some point k_* in the 1BZ. By π PH symmetry, relation (5) it also vanishes at $\pi - k_*$. The sign of the vertical component ε_k at k_* and $\pi - k_*$ are opposite as the \cos functions appearing in vertical component ε_k of Anderson pseudovector change sign upon going from k_* to $\pi - k_*$ when r is odd.

Now starting from the XY model ($p = 0$) and focusing only in the right half of 1BZ with $k > 0$, at $k = 0$ and $k = \pi$ the Anderson vectors point to north and south poles respectively (Fig. 2-b) which means that in the right half of 1BZ one picks up a half-integer winding. For every k_* if the winding vector points to some pole the one at $\pi - k_*$ will point to opposite pole, corresponding to every pair of roots $k_*, \pi - k_*$ of Δ_k , an integer winding is inserted to the right half of 1BZ. This means that always half-integer windings are possible in the right half of 1BZ. Therefore the winding number picked over the whole 1BZ is an odd number. That is why in the right panel of Fig. 3 we only have odd winding numbers. The fact that for odd r , only even number of MFs and only odd n_W s are possible is consistent with Eq. (13). This line of reasoning implies that in the simple case $p = 0$ corresponding to XY (or Kitaev) chain, by π PH symmetry the topologically non-trivial phase always hosts two independent Majorana end modes re-

lated by $A_j \leftrightarrow -(-1)^j A_j$.

It can be noticed that the Z_2 index defined by $\nu = \text{sign}(\varepsilon_0)\text{sign}(\varepsilon_\pi)$ ¹², gives $\nu = -1$ when r is odd. However, when r is even, $\nu = \text{sign}(|J_r/J_1| - 1)$. For even r , the $\nu = +1(-1)$ corresponds to even (odd) values of n_W . The physical interpretation of ν is as follows: When $\nu = +1(-1)$ the identity of Bogolons does not change (changes) from hole-like to particle-like when k spans the range $[0, \pi]$. The presence of π PH symmetry for odd r guarantees that the above Z_2 index takes only one value -1 which means that the charge character of Bogolons at $k = 0$ and $k = \pi$ are opposite. Breaking π PH allows for both ± 1 values.

Summary. To summarize, we have presented an exactly solvable extension of the quantum XY model that involves clusters of $n = r + 1$ spins interacting at range r . The ensuing JW representation is a topological superconductor in BDI class. We showed that the TR operation of original spin variables translates to a sliding PH transformation of JW fermions, π PH. The presence of π PH implies that corresponding to every MF wave function A_j , there is a partner MF whose wave function is $-(-1)^j A_j$ which in turn restricts the number of MFs to even values only. The π PH also implies that the roots of pairing potential come in pairs which restricts the Z winding numbers to odd integers only. The Bott periodicity¹¹ implies that there should exist similar restriction in higher dimensions on topological invariants when π PH is a symmetry. It will be interesting to study possible higher dimensional models with π PH symmetry in electronic systems^{16,18,19}. The number n_M of MFs leaves a unique signature in tunneling experiments and hence remains directly accessible to experiments. Array of magnetic nano-particles on a superconductor is described by an effective theory that includes $r = 2$ hopping between the spinless fermions^{10,20} which may serve as potential platform to materialize 3XY model.

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